

An Extended Pruess Method for Sturm-Liouville Problems

Robert Carlson
Department of Mathematics
University of Colorado at Colorado Springs
carlson@math.uccs.edu

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Abstract

A new version of the piecewise approximation (Pruess) method is developed for calculating eigenvalues of Sturm-Liouville problems. The usual piecewise constant or piecewise linear potential approximations are replaced by translates of $2/\cos^2(x)$, whose corresponding eigenvalue equation has elementary solutions.

Keywords: Sturm-Liouville problem, Pruess method, eigenvalue computations.

AMS subject classification: 34L16, 65L15

1 Introduction

The basic Sturm-Liouville problem asks for the eigenvalues and eigenfunctions of the second order linear equation

$$-y'' + p(x)y = \lambda y, \quad 0 \leq x \leq 1, \quad (1.1)$$

satisfying the separated boundary conditions

$$a_0 y(0) + a_1 y'(0) = 0, \quad b_0 y(1) + b_1 y'(1) = 0. \quad (1.2)$$

The constants a_j, b_j should be real, and not both zero at either endpoint. The potential $p(x)$ should be real valued; although singular potentials are interesting, our examples will be continuous. A closely related problem asks for periodic eigenfunctions and the associated eigenvalues, with the boundary conditions

$$y(0) = y(1), \quad y'(0) = y'(1). \quad (1.3)$$

The book [13] provides a systematic account of numerical methods for solving Sturm-Liouville problems.

Popular algorithms known as piecewise constant midpoint methods, or Pruess methods, are based on a piecewise constant approximation $\tilde{p}(x)$ of the coefficient $p(x)$. This algorithmic theme was introduced in [2] and eventually developed into well analyzed packages [7, 8, 9, 12]. When \tilde{p} is piecewise constant, the solutions of (1.1) have a simple piecewise description in terms of the trigonometric functions $\cos(x), \sin(x)$. Taking advantage of the simple explicit formulas for the basis, a shooting method can provide an efficient algorithm for accurately computing eigenvalues and eigenfunctions.

Piecewise constant approximations are rather crude, so it is not surprising that more refined approximations were considered. Piecewise polynomial approximations were analyzed in [11], but the convenient basis of solutions is generally absent, making corresponding algorithms much less attractive. These difficulties are reduced for piecewise linear approximation [5, 6] because the bases can be expressed efficiently in terms of Airy functions.

This work considers a different type of piecewise approximation, focusing on the existence of an elementary basis of solutions to (1.1). By using commutation methods, also known as Darboux transformations, it is possible to find examples of (1.1) with nonconstant coefficients whose solutions are elementary functions for all values of λ . A well-known example is

$$-y'' + \frac{2}{x^2}y = \lambda y, \quad (1.4)$$

which has solutions

$$y_1(x, \lambda) = \sin(\sqrt{\lambda}x) + \frac{\cos(\sqrt{\lambda}x)}{\sqrt{\lambda}x}, \quad y_2(x, \lambda) = \cos(\sqrt{\lambda}x) - \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}x}. \quad (1.5)$$

The existence of such examples suggests that certain nonpolynomial piecewise approximations of $p(x)$ in (1.1) might provide an extension of the piecewise constant Pruess method with better approximation of $p(x)$, elementary expressions for the solutions, and more efficient computation of the eigenvalues.

This work describes such an algorithm and reports on its performance in a number of numerical experiments. The piecewise approximations of the extended algorithm have the form

$$p_k(x) = \alpha_k + \frac{2}{\cos^2(x - \xi_k)}, \quad x_k \leq x < x_{k+1}, \quad (1.6)$$

taking advantage of the fact that the equation

$$-y'' + \frac{2}{\cos^2(x)}y = \lambda y \quad (1.7)$$

has a basis of solutions Y_1, Y_2 with

$$\begin{aligned} Y_1(x, \lambda) &= \cos(\sqrt{\lambda}x) + \tan(x) \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}, \\ Y_2(x, \lambda) &= \frac{1}{1 - \lambda} \tan(x) \cos(\sqrt{\lambda}x) - \frac{\lambda}{1 - \lambda} \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}, \\ Y_1'(x, \lambda) &= \tan(x) \cos(\sqrt{\lambda}x) + \left[\frac{1}{\cos^2(x)} - \lambda \right] \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}, \\ Y_2'(x, \lambda) &= \left[\frac{1}{\cos^2(x)} - \lambda \right] \frac{\cos(\sqrt{\lambda}x)}{1 - \lambda} - \frac{\lambda}{1 - \lambda} \tan(x) \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}. \end{aligned} \quad (1.8)$$

On the interval $(-\pi/2, \pi/2)$ the derivative values of $2/\cos^2(x)$ increase monotonically from $-\infty$ to ∞ . For each subinterval $[x_k, x_{k+1}]$ our algorithm computes a derivative estimate for $p(x)$, then selects ξ_k in (1.6) to match the estimate. The constant α_k is then adjusted to optimize the nearly linear local approximation.

The subsequent sections describe the background ideas, give a description of the algorithm, and report on its performance. After a review of piecewise approximations of (1.1) and the corresponding transition matrices, the general commutation method is considered. Examples are provided. When the examples are more complex than (1.7) the formulas for solutions to the eigenvalue equation (1.1) quickly grow in complexity; the properties of the corresponding potentials are hard to discern. The extended algorithm presented here uses (1.7); it produces a piecewise approximation of $p(x)$ which is nearly linear, but with solutions which are elementary functions instead of Airy functions.

Algorithm accuracy was compared for several variants of both the piecewise constant Pruess method and the new algorithm. For both methods the sample points were chosen in two ways: uniformly spaced, and adaptively chosen to optimize piecewise approximation. The lowest 25 eigenvalues were computed for five regular Sturm-Liouville problems. The reported data comprises eigenvalues 1, 2, 3, 12 and 25. The lowest eigenvalues typically show the largest errors. While the new algorithm does quite well in approximation of the potentials, all of the algorithms had similar performance for computation of the eigenvalues. As long as eigenvalue computation is the goal, the simplicity and speed of the piecewise constant Pruess method make it preferable.

2 The basic idea

Suppose the interval $[0, 1]$ is partitioned into K subintervals with endpoints $0 = x_0 < x_1 < \dots < x_K = 1$. Assume that the function $p(x)$ from (1.1) has a piecewise definition based on this partition,

$$p(x) = p_k(x), \quad x_k \leq x < x_{k+1}, \quad k = 0, \dots, K-1.$$

The functions $p_k(x)$ are assumed to have a continuous extension to the closed interval $[x_k, x_{k+1}]$. On each subinterval there is a basis $y_k(x, \lambda), z_k(x, \lambda)$ of solutions to (1.1) satisfying the initial conditions

$$\begin{aligned} y_k(x_k, \lambda) &= 1, & y'_k(x_k, \lambda) &= 0, \\ z_k(x_k, \lambda) &= 0, & z'_k(x_k, \lambda) &= 0. \end{aligned}$$

It will be convenient to package these functions into a matrix

$$\begin{pmatrix} y_k(x, \lambda) & z_k(x, \lambda) \\ y'_k(x, \lambda) & z'_k(x, \lambda) \end{pmatrix} \tag{2.1}$$

Because $p_0(x)$ has a continuous extension to the closed interval $[x_0, x_1]$, the solutions y_0, z_0 extend to x_1 , prescribing initial data

$$\begin{pmatrix} y(x_1, \lambda) & z(x_1, \lambda) \\ y'(x_1, \lambda) & z'(x_1, \lambda) \end{pmatrix} = \begin{pmatrix} y_0(x_1, \lambda) & z_0(x_1, \lambda) \\ y'_0(x_1, \lambda) & z'_0(x_1, \lambda) \end{pmatrix},$$

for the continuation to the next interval, where the solution matching values and derivatives at x_1 takes the form

$$\begin{pmatrix} y(x, \lambda) & z(x, \lambda) \end{pmatrix} = \begin{pmatrix} y_1(x, \lambda) & z_1(x, \lambda) \end{pmatrix} \begin{pmatrix} y_0(x_1, \lambda) & z_0(x_1, \lambda) \\ y'_0(x_1, \lambda) & z'_0(x_1, \lambda) \end{pmatrix}.$$

By induction we find that the values and derivatives of y and z at 1 are given by the product of matrices,

$$\begin{pmatrix} y(1, \lambda) & z(1, \lambda) \\ y'(1, \lambda) & z'(1, \lambda) \end{pmatrix} = \prod_{k=0}^{K-1} T_k(\lambda), \quad T_k(\lambda) = \begin{pmatrix} y_k(x_{k+1}, \lambda) & z_k(x_{k+1}, \lambda) \\ y'_k(x_{k+1}, \lambda) & z'_k(x_{k+1}, \lambda) \end{pmatrix},$$

where the factors in the product have indices decreasing from left to right,

$$\prod_{k=0}^{K-1} T_k(\lambda) = T_{K-1}(\lambda) \cdots T_1(\lambda) T_0(\lambda), \quad (2.2)$$

The piecewise constant approximation methods use $p_k(x) = \alpha_k$. If $l_k = x_{k+1} - x_k$, the matrices T_k then have the elementary form

$$T_k(\lambda) = \begin{pmatrix} \cos(l_k \sqrt{\lambda - \alpha_k}) & \sin(l_k \sqrt{\lambda - \alpha_k}) / \sqrt{\lambda - \alpha_k} \\ -\sqrt{\lambda - \alpha_k} \sin(l_k \sqrt{\lambda - \alpha_k}) & \cos(l_k \sqrt{\lambda - \alpha_k}) \end{pmatrix}. \quad (2.3)$$

The next section will discuss the construction of model potentials leading to roughly linear piecewise approximations of the potential $p(x)$ which retain elementary (but more complex) formulas for the matrices $T_k(\lambda)$.

3 Commutation methods

It is possible to generate a large collection of differential operators whose eigenvalue equations (1.1) have elementary solutions like (1.8). These operators and their solutions are generated from the case $p(x) = 0$ using the commutation method, also known as a Darboux transformation. Such ideas have been used repeatedly in the past [1], [3], [4, p. 425-444], [10, p. 88-91].

3.1 General idea

Suppose L_0 is a second order operator of the form $L_0 = -D^2 + p_0$, and y_1 is a nontrivial solution of

$$(L_0 - \mu_1)y = 0.$$

Then $L_0 - \mu_1$ may be factored,

$$L_0 - \mu_1 = F_- F_+, \quad F_{\pm} = \pm D - \frac{y_1'}{y_1}, \quad p_0 - \mu_1 = \left(\frac{y_1'}{y_1}\right)' + \left(\frac{y_1'}{y_1}\right)^2.$$

If z satisfies a second eigenvalue equation $L_0 z = \lambda z$, then $(F_- F_+ + \mu_1)z = \lambda z$. Applying F_+ to both sides gives

$$[F_+ F_- + \mu_1]F_+ z = \lambda F_+ z,$$

so that the new operator $L_1 = -D^2 + p_1$ has a solution $F_+ z$ for the eigenvalue equation $L_1 F_+ z = \lambda F_+ z$, where

$$L_1 = F_+ F_- + \mu_1 = -D^2 - \left(\frac{y_1'}{y_1}\right)' + \left(\frac{y_1'}{y_1}\right)^2 + \mu_1 = -D^2 - p_0 + 2\mu_1 + 2\left(\frac{y_1'}{y_1}\right)^2. \quad (3.1)$$

That is

$$p_1 = -p_0 + 2\mu_1 + 2\left(\frac{y_1'}{y_1}\right)^2.$$

Notice too that if $\lambda \neq \mu_1$, then the linear map $z \rightarrow F_+ z$ is invertible since

$$\begin{pmatrix} F_+ z \\ (F_+ z)' \end{pmatrix} = A \begin{pmatrix} z \\ z' \end{pmatrix}, \quad A = \begin{pmatrix} -y_1'/y_1 & 1 \\ p - \lambda - (y_1'/y_1)' & -y_1'/y_1 \end{pmatrix},$$

with $\det(A) = \lambda - \mu_1$.

If $\mu_2 \neq \mu_1$ the process may be repeated. Adding parameters for clarity, the mapping on z is given by

$$F_+(\mu_1, \mu_2)z(\lambda) = \left[D - \frac{(F_+(\mu_1)y_2(\mu_2))'}{F_+(\mu_1)y_2(\mu_2)} \right] F_+(\mu_1)z.$$

The operator $F_+(\mu_1, \mu_2)$, which is second order with leading coefficient 1, annihilates $y_1(\mu_1)$ and $y_2(\mu_2)$, so

$$F_+(\mu_1, \mu_2)z = \frac{1}{y_1(\mu_1)y_2'(\mu_2) - y_1'(\mu_1)y_2(\mu_2)} \det \begin{pmatrix} z & y_1 & y_2 \\ z' & y_1' & y_2' \\ z'' & y_1'' & y_2'' \end{pmatrix}. \quad (3.2)$$

Notice that $F_+(\mu_1, \mu_2) = F_+(\mu_2, \mu_1)$, and this construction extends to maps $F_+(\mu_1, \dots, \mu_n)$, with

$$F_+(\mu_1, \dots, \mu_n)z \quad (3.3)$$

$$= (-1)^n \det \begin{pmatrix} y_1 & \cdots & y_n \\ \vdots & \cdots & \vdots \\ y_1^{(n-1)} & \cdots & y_n^{(n-1)} \end{pmatrix}^{-1} \det \begin{pmatrix} z & y_1 & \cdots & y_n \\ z^{(1)} & y_1^{(1)} & \cdots & y_n^{(1)} \\ \vdots & \vdots & \cdots & \vdots \\ z^{(n)} & y_1^{(n)} & \cdots & y_n^{(n)} \end{pmatrix}.$$

The operators $-D^2 + p_n$ resulting from an n -th commutation of the initial operator $-D^2 + p_0$ have a recursive description. For the n -th commutation, a solution of $(-D^2 + p_{n-1})y = \mu_n y$ has the form $z_n = F_+(\mu_1, \dots, \mu_{n-1})y_n$ where $(-D^2 + p_0)y_n = \mu_n y_n$. From (3.1) we see that the n -th commutation results in a new potential

$$p_n = -\left(\frac{z'_n}{z_n}\right)' + \left(\frac{z'_n}{z_n}\right)^2 + \mu_n = -p_{n-1} + 2\mu_n + 2\left(\frac{z'_n}{z_n}\right)^2. \quad (3.4)$$

Suppose the coefficient p_0 is continuous on $[\alpha, \beta]$. If $y_1(\mu_1)$ has a zero on this interval then $F_+(\mu_1)$ and the modified operator (3.1) will have singularities. The situation is different for the double commutation (3.2). Notice that $F_+(\mu_1, \mu_2)$ is defined when $\mu_1 = \mu_2$ if $y_1(\mu_1)$ and $y_2(\mu_2)$ are linearly independent. In this case $F_+(\mu_1, \mu_1)$ agrees with $L - \mu_1$ and the operator is not altered. The transformed operator will remain nonsingular on $[\alpha, \beta]$ if $y_2(\mu_2)$ is sufficiently close to $y_2(\mu_1)$.

3.2 Elementary single commutation

If $p_0 = 0$ and $y_1 = \cos(\sqrt{\mu_1}x)$, then

$$F_+ \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}} = \cos(\sqrt{\lambda}x) + \sqrt{\mu_1} \tan(\sqrt{\mu_1}x) \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}$$

and

$$F_+ \cos(\sqrt{\lambda}x) = -\lambda \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}} + \sqrt{\mu_1} \tan(\sqrt{\mu_1}x) \cos(\sqrt{\lambda}x)$$

are solutions of

$$[-D^2 + \frac{2\mu_1}{\cos^2(\sqrt{\mu_1}x)}]Y = \lambda Y, \quad p_1 = \frac{2\mu_1}{\cos^2(\sqrt{\mu_1}x)}. \quad (3.5)$$

Assuming that $\sqrt{\mu_1} > 0$, the derivative of $p_1(x)$ increases monotonically from $-\infty$ to ∞ on the interval $(-\frac{\pi}{2\sqrt{\mu_1}}, \frac{\pi}{2\sqrt{\mu_1}})$. Simple calculations give

$$\frac{d}{dx} \frac{2\mu_1}{\cos^2(\sqrt{\mu_1}x)} = 4\mu_1^{3/2} \tan(\sqrt{\mu_1}x)[1 + \tan^2(\sqrt{\mu_1}x)]$$

and

$$\begin{aligned} \frac{d^2}{dx^2} \frac{2\mu_1}{\cos^2(\sqrt{\mu_1}x)} &= 4\mu_1^2 \sec^2(\sqrt{\mu_1}x)[1 + 3\tan^2(\sqrt{\mu_1}x)] \\ &= 4\mu_1^2[1 + \tan^2(\sqrt{\mu_1}x)][1 + 3\tan^2(\sqrt{\mu_1}x)] \end{aligned}$$

Notice that the second derivative is always positive, so a richer family of examples would be needed to locally match first and second derivatives of a potential $p(x)$.

In case $\sqrt{\mu_1} = 1$, a basis for $L_1 y = \lambda y$ is given by (1.8). If $y_1 = \sin(\sqrt{\mu_1}x)$ instead of $y_1 = \cos(\sqrt{\mu_1}x)$, then

$$\frac{y_1'}{y_1} = \frac{\sqrt{\mu_1} \cos(\sqrt{\mu_1}x)}{\sin(\sqrt{\mu_1}x)}, \quad p_1 = 2\mu_1 + 2\left(\frac{y_1'}{y_1}\right)^2 = \frac{2\mu_1}{\sin^2(\sqrt{\mu_1}x)}.$$

Notice that $p_1 = 2/x^2$ when $\mu_1 = 0$. Repeated commutations can generate potentials $q_m(x) = \frac{m(m+1)}{x^2}$ for $m = 1, 2, 3, \dots$. These cases are closely related to Bessel's equation of half integer order $\nu = (2m+1)/2$; see [14, p.364-365] for some explicit formulas.

3.3 Elementary double commutation

Since single commutation leads to potentials with constrained second derivatives, it is natural to consider examples generated by repeated commutations. The formulas quickly become unwieldy. A double commutation can be based on

$$z_2 = \sqrt{\mu_2} \cos(\sqrt{\mu_2}x) + \sqrt{\mu_1} \tan(\sqrt{\mu_1}x) \sin(\sqrt{\mu_2}x)$$

with

$$\begin{aligned} z_2' &= -\mu_2 \sin(\sqrt{\mu_2}x) \\ &+ \mu_1 \sec^2(\sqrt{\mu_1}x) \sin(\sqrt{\mu_2}x) + \sqrt{\mu_1} \sqrt{\mu_2} \tan(\sqrt{\mu_1}x) \cos(\sqrt{\mu_2}x). \end{aligned}$$

Transformation of (3.5) results in the new operators $L_2 = -D^2 + p_2$ with

$$p_2 = \frac{-2\mu_1}{\cos^2(\sqrt{\mu_1}x)} + 2\mu_2 \tag{3.6}$$

$$+2 \tan^2(\sqrt{\mu_2}x) \left[\frac{(\mu_1 - \mu_2) + \mu_1 \tan^2(\sqrt{\mu_1}x) + \sqrt{\mu_1} \sqrt{\mu_2} \tan(\sqrt{\mu_1}x) \cot(\sqrt{\mu_2}x)}{\sqrt{\mu_2} + \sqrt{\mu_1} \tan(\sqrt{\mu_1}x) \tan(\sqrt{\mu_2}x)} \right]^2.$$

4 Algorithm description

4.1 Table development

The computations are based on the potential

$$q(x) = \frac{2}{\cos^2(x)}, \quad q'(x) = \frac{4 \sin(x)}{\cos^3(x)} = 4 \tan(x) [1 + \tan^2(x)].$$

On a subinterval interval $[x_k, x_{k+1}] \subset [0, 1]$ with midpoint $m_k = (x_k + x_{k+1})/2$ the full model potential will have the form

$$\alpha_k + \frac{2}{\cos^2(x - m_k + z_k)}.$$

The point z_k is chosen so that $q'(z_k)$ approximates $p'(m_k)$. The selection of z_k is based on a table of 201 samples $((q')^{1/3}(t_j), t_j)$, with $q'(t_j)$ in the range $[-1000, 1000]$. The cube root was selected to provide adequate sampling for moderate values of q' .

A fixed number N of sample points $0 \leq x_k \leq 1$ were selected. Some trials used uniformly spaced samples for both the piecewise constant Pruess method and the extended method. Another set of samples was selected to minimize

$$\sum_{k=0}^{N-1} \int_{x_k}^{x_{k+1}} (p(x) - p(m_k))^2 dx \quad (4.1)$$

for the Pruess method. For the new method a set of samples was selected based on a piecewise linear approximation, the samples chosen to minimize

$$\sum_{k=0}^{N-1} \int_{x_k}^{x_{k+1}} (p(x) - [P'_k(x - m_k) + p(m_k)])^2 dx, \quad P'_k = \frac{p(x_{k+1}) - p(x_k)}{x_{k+1} - x_k}. \quad (4.2)$$

After the selection of sample points x_k , the values P'_k are also used to select the points z_k where $q'(z_k) \simeq p'(m_k)$. The points z_k are computed by combining linear interpolation with the table values discussed above. The constants

$$\alpha_k = p(m_k) - 2[\tan(m_k + z_k) - \tan(z_k - m_k)]/L_k.$$

are chosen so that the model potential on $[x_k, x_{k+1}]$ has the same integral as given by the midpoint rule.

Having selected x_k, z_k, α_k , the equation which locally approximates

$$-y'' + p(x)y = \lambda y$$

on the interval $[x_k, x_{k+1}]$ is

$$-y'' + \left[\frac{2}{\cos^2(x - m_k + z_k)} + \alpha_k \right] y = \lambda y,$$

or

$$-y'' + \frac{2}{\cos^2(x - m_k + z_k)} y = \sigma y, \quad \sigma = \lambda - \alpha_k.$$

Using (1.8), this equation has a basis of solutions $Y_1(x - m_k + z_k, \sigma), Y_2(x - m_k + z_k, \sigma)$. After converting to the basis (W_1, W_2) satisfying

$$\begin{pmatrix} W_1 & W_2 \\ W_1' & W_2' \end{pmatrix} (x_k, \lambda) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

and letting $l_k = x_{k+1} - x_k$, the transition matrix T_k will be

$$T_k(\lambda) = \begin{pmatrix} Y_1 & Y_2 \\ Y_1' & Y_2' \end{pmatrix} (x_{k+1} - m_k + z_k, \sigma) \begin{pmatrix} Y_2' & -Y_2 \\ -Y_1' & Y_1 \end{pmatrix} (z_k - \frac{l_k}{2}, \sigma).$$

Although the evaluation of $T_k(\lambda)$ in the extended method is not computationally expensive, the evaluation (2.3) for piecewise constant approximations is more efficient. The total algorithm ran about three times as fast for the 16 subinterval cases if the piecewise constant approximation was used instead of the extended algorithm.

Trials were run for regular Sturm-Liouville problems on the interval $[0, 1]$ using the Dirichlet boundary conditions $y(0) = 0 = y(1)$. Extensive theoretical studies [10] of these problems are available. The eigenvalues are simple, and typically well separated. The algorithm used initial samples of the eigenvalue parameter expected to be considerable closer than the actual eigenvalues. A bisection method searched for roots of $W_2(1, \lambda)$, giving the Dirichlet eigenvalues.

5 Performance

The following five potentials were tested:

$$(1) \ p(x) = \frac{\pi^2}{(\pi x + 0.1)^2},$$

$$(2) \ p(x) = 1 + \cos(\pi t) + 5 \cos(2\pi t) - 2 \cos(3\pi t) - 3 \cos(4\pi t), \quad t = x - 0.5,$$

$$(3) \ p(x) = \begin{cases} x \sin(1/x), & x \geq 10^{-6}, \\ 0, & x < 10^{-6} \end{cases},$$

$$(4) \ p(x) = \frac{1}{\cos(x)^2}, \quad (5) \ p(x) = \frac{1}{.2 + \sqrt{x(1-x)}}.$$

In all cases, $0 \leq x \leq 1$ and the Dirichlet boundary conditions $y(0) = 0 = y(1)$ were used.

The first 25 eigenvalues were computed. The main experiments compared the performance of several algorithms when the unit interval was partitioned with 16 subintervals. Performance was assessed by comparing the computed eigenvalues with the results obtained from the Pruess method (U-P128) using 128 subintervals of equal length. Case 1 was used to test the accuracy of U-P128. This case, considered to be challenging, is a rescaling to $[0, 1]$ of a problem in Appendix A of [13]. The rescaling means the numbers calculated here should agree with [13] after division by π^2 . A comparison showed a maximum difference of 4 in the least significant (fifth) digit of the second eigenvalue. The other eigenvalues shown here had a difference of 1 in the least significant digit.

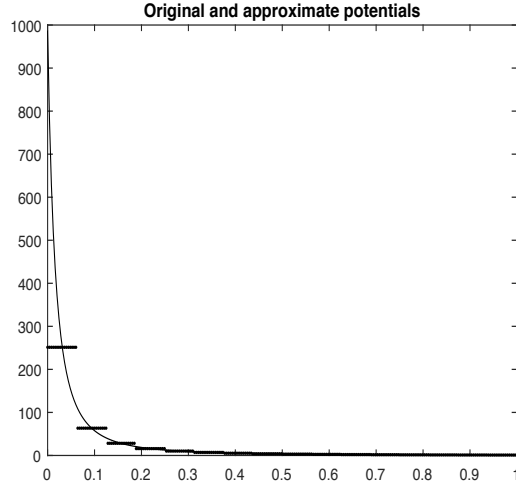
The tables and figures below show a sampling of results. The figures show plots of the potential $p(x)$ and either the 16 equal length subinterval piecewise constant approximation, or the extended method with 16 subintervals, with sample points chosen to minimize the penalty of (4.2). In each case there are six trials. The trials labelled U-P 16, U-P 32, and U-P 128 used the piecewise constant Pruess method with 16, 32, and 128 equal length subintervals respectively. The trial labelled A-P 16 used 16 subintervals, with sample points chosen to minimize the penalty of (4.1). The trial U-X 16 used the extended method with 16 equal length subintervals. The trial A-X 16 used the extended method with 16 subintervals, with sample points chosen to minimize the penalty of (4.2).

The tables show the values of 5 eigenvalues: the first three, number 12 and number 25. For these methods the smaller eigenvalues are more challenging

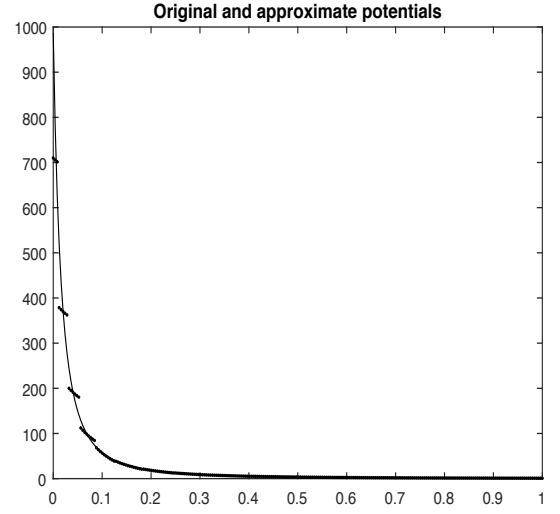
than the larger ones. The U-P 32 algorithm is included as an indication of the improvement when the number of equal length subintervals is doubled. The bottom of the table indicates which of the 16 subinterval algorithms was most accurate. Overall the performances were similar.

The extended algorithm generally did a good job providing a piecewise approximation of the potential. If such an approximation were the main goal, the extended Pruess algorithm would be attractive, but if the main goal is computation of the eigenvalues, the piecewise constant Pruess method seems a clear winner because of its simplicity and speed.

Case 1



Pruess method, uniform sampling

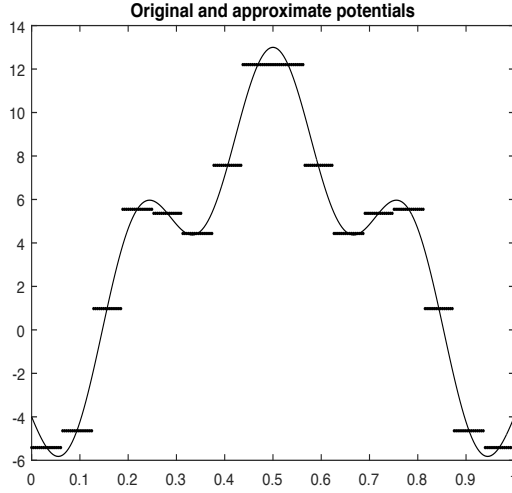


Extended method, adaptive sampling

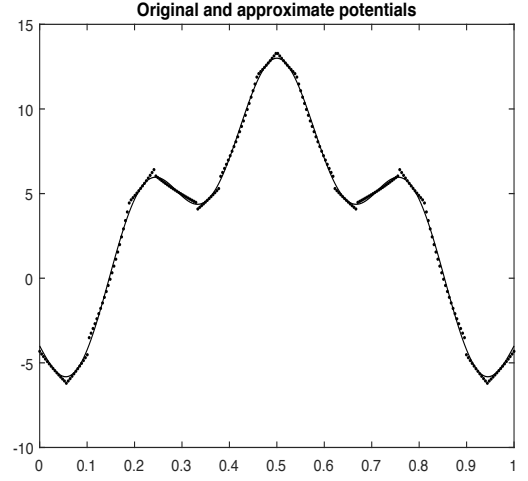
Case 1:

	λ_1	λ_2	λ_3	λ_{12}	λ_{25}
$U - P_{128}$	$1.5001e1$	$4.8792e1$	$1.0151e2$	$1.4466e3$	$6.1974e3$
$U - P_{32}$	$1.5015e1$	$4.8848e1$	$1.0164e2$	$1.4477e3$	$6.1990e3$
$U - P_{16}$	$1.5055e1$	$4.9017e1$	$1.0202e2$	$1.4491e3$	$6.1938e3$
$U - X_{16}$	$1.4938e1$	$4.8600e1$	$1.0145e2$	$1.4483e3$	$6.1938e3$
$A - P_{16}$	$1.5031e1$	$4.8930e1$	$1.0191e2$	$1.4494e3$	$6.1942e3$
$A - X_{16}$	$1.4940e1$	$4.8626e1$	$1.0127e2$	$1.4463e3$	$6.1969e3$
<i>best 16</i>	$A - P$	$A - P$	$U - X$	$A - X$	$A - X$

Case 2



Pruess method, uniform sampling

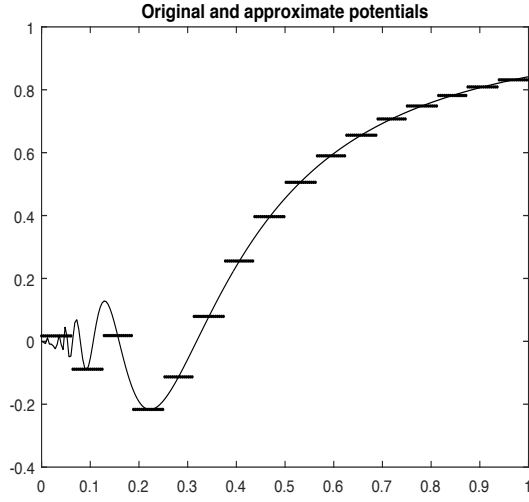


Extended method, adaptive sampling

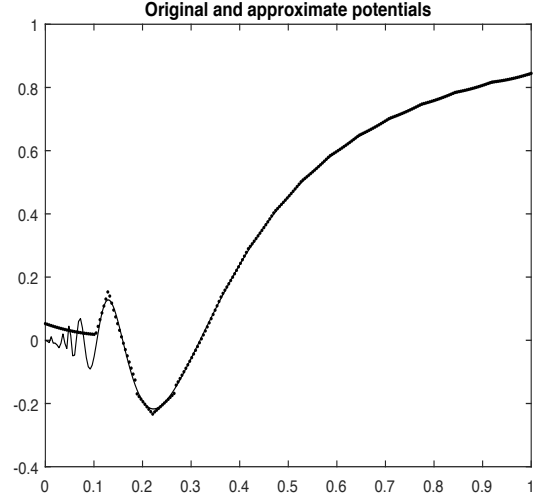
Case 2:

	λ_1	λ_2	λ_3	λ_{12}	λ_{25}
$U - P128$	$1.6656e1$	$4.3260e1$	$9.3189e1$	$1.4245e3$	$6.1718e3$
$U - P32$	$1.6651e1$	$4.3257e1$	$9.3176e1$	$1.4245e3$	$6.1718e3$
$U - P16$	$1.6635e1$	$4.3247e1$	$9.3135e1$	$1.4247e3$	$6.1718e3$
$U - X16$	$1.6678e1$	$4.3273e1$	$9.3235e1$	$1.4245e3$	$6.1718e3$
$A - P16$	$1.6638e1$	$4.3175e1$	$9.3188e1$	$1.4245e3$	$6.1718e3$
$A - X16$	$1.6664e1$	$4.3271e1$	$9.3199e1$	$1.4245e3$	$6.1718e3$
$best\ 16$	$A - X$	$A - X$	$A - P$	—	—

Case 3



Pruess method, uniform sampling

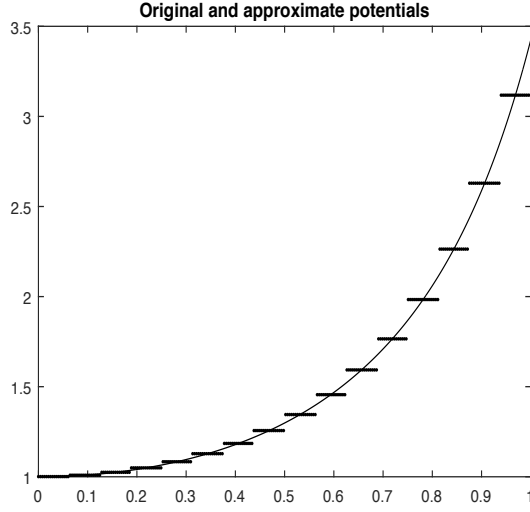


Extended method, adaptive sampling

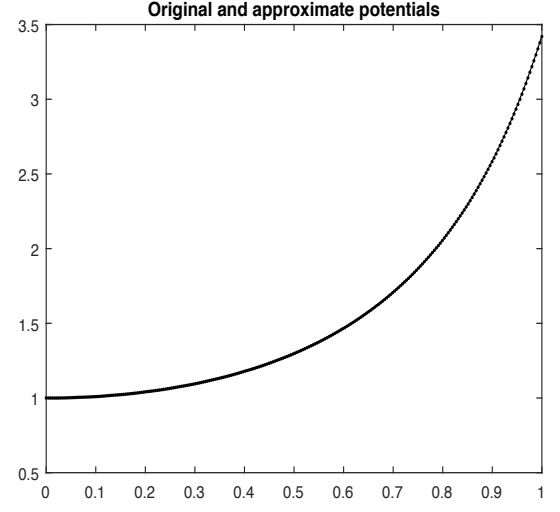
Case 3:

	λ_1	λ_2	λ_3	λ_{12}	λ_{25}
$U - P_{128}$	1.0250e1	3.9820e1	8.9210e1	1.4216e3	6.1689e3
$U - P_{32}$	1.0250e1	3.9821e1	8.9212e1	1.4216e3	6.1689e3
$U - P_{16}$	1.0249e1	3.9818e1	8.9204e1	1.4216e3	6.1689e3
$U - X_{16}$	1.0249e1	3.9816e1	8.9204e1	1.4216e3	6.1689e3
$A - P_{16}$	1.0248e1	3.9815e1	8.9202e1	1.4216e3	6.1689e3
$A - X_{16}$	1.0250e1	3.9821e1	8.9214e1	1.4216e3	6.1689e3
<i>best 16</i>	$A - X$	$A - X$	$A - X$	—	—

Case 4



Pruess method, uniform sampling

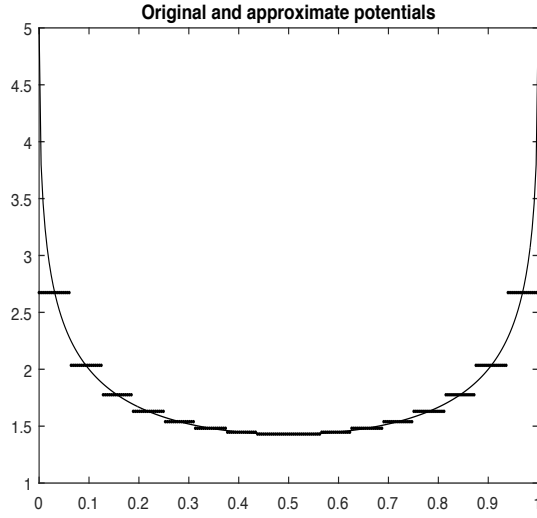


Extended method, adaptive sampling

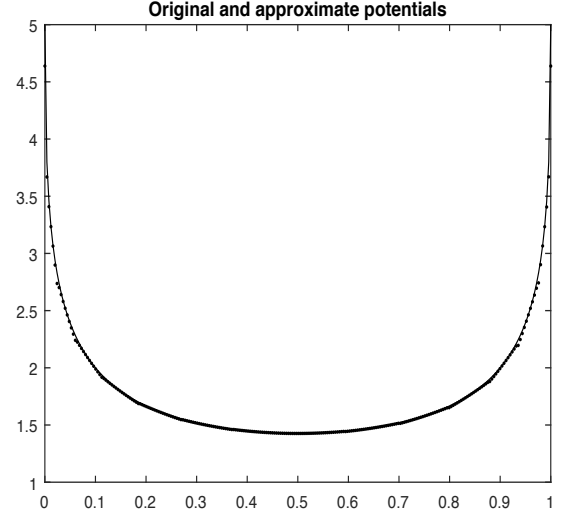
Case 4:

	λ_1	λ_2	λ_3	λ_{12}	λ_{25}
$U - P128$	1.1255e1	4.0979e1	9.0357e1	1.4228e3	6.1701e3
$U - P32$	1.1256e1	4.0980e1	9.0357e1	1.4228e3	6.1701e3
$U - P16$	1.1256e1	4.0981e1	9.0359e1	1.4228e3	6.1701e3
$U - X16$	1.1254e1	4.0978e1	9.0355e1	1.4228e3	6.1701e3
$A - P16$	1.1256e1	4.0980e1	9.0357e1	1.4228e3	6.1701e3
$A - X16$	1.1254e1	4.0978e1	9.0356e1	1.4228e3	6.1701e3
$best - 16$	—	—	$A - P$	—	—

Case 5



Pruess method, uniform sampling



Extended method, adaptive sampling

Case 5:

	λ_1	λ_2	λ_3	λ_{12}	λ_{25}
$U - P_{128}$	1.1385e1	4.1111e1	9.0504e1	1.4230e3	6.1703e3
$U - P_{32}$	1.1385e1	4.1111e1	9.0506e1	1.4230e3	6.1703e3
$U - P_{16}$	1.1386e1	4.1114e1	9.0510e1	1.4230e3	6.1703e3
$U - X_{16}$	1.1382e1	4.1102e1	9.0488e1	1.4229e3	6.1703e3
$A - P_{16}$	1.1384e1	4.1108e1	9.0504e1	1.4230e3	6.1703e3
$A - X_{16}$	1.1382e1	4.1106e1	9.0499e1	1.4230e3	6.1703e3
<i>best 16</i>	<i>P</i>	<i>P</i>	<i>A - P</i>	—	—

References

- [1] J. Burchnall and T. Chaundy. *Commutative ordinary differential operators* Proc. London Math. Soc. 21 (1922), 420-440.
- [2] J. Canosa and R. Gomes De Oliveira. *A new method for the solution of the Schrödinger equation* Journal of Computational Physics 5 (1970), 188-207.
- [3] R. Carlson. *Construction of isospectral deformations of differential operators with periodic coefficients* Journal of Functional Analysis 46 (1982), 265-279.
- [4] F. Gesztesy and H. Holden. *Soliton Equations and Their Algebraic-Geometric Solutions: volume 1*. Cambridge University Press, 2003.
- [5] V. Ledoux. *Study of Special Algorithms for solving Sturm-Liouville and Schrödinger equations* Universiteit Gent (2006-7).
- [6] V. Ledoux, M. Rizea, L. Ixaru, G. Vanden Berghe, M. Van Daele. *Solution of the Schrödinger equation by a high order perturbation method based on a linear reference potential* Computer Physics Communications 175 (2006), 424-439.
- [7] V. Ledoux, M. Van Daele, GS. Vanden Berghe. *Efficient computation of high index Sturm-Liouville eigenvalues for problems in physics* Computer Physics Communications 180 (2009), 241-250.
- [8] V. Ledoux, M. Van Daele. *Solving Sturm-Liouville problems by piecewise perturbation methods, revisited* Computer Physics Communications 181 (2010), 1335-1345.
- [9] M. Marletta. *Automatic Solution of Sturm-Liouville problems using the Pruess method* Journal of Computational and Applied Mathematics 39 (1992), 57-78.
- [10] J. Pöschel and E. Trubowitz. *Inverse Spectral Theory* Academic Press, Orlando, 1987
- [11] S. Pruess. *Estimating the Eigenvalues of Sturm-Liouville Problems by Approximating the Differential Equation* SIAM J. Numer. Anal. 10 (1) (1973), 55-68.

- [12] S. Pruess and C. Fulton. *Mathematical Software for Sturm-Liouville problems* ACM Transactions on Mathematical Software 19 (3) (1993), 360-376.
- [13] J. Pryce. *Numerical Solution of Sturm-Liouville Problems*. Oxford University Press, 1993.
- [14] E. Whittaker and G. Waston. *A Course of Modern Analysis*. Cambridge, 1990.